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Abstract The equations governing the conditions of mechanical equilibrium in fluid membranes subject to bending are revisited thanks to the principle of virtual work. The note proposes systematic tools to obtain the shape equation and the line condition instead of Christoffel symbols and the complex calculations they entail. The method seems adequate to investigate all problems involving surface energies.

Keywords Vesicles, surface energy, differential geometry of surfaces, shape equation.

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Mathematics Subject Classification (2000) 74K15, 76Z99, 92C37.

1 Introduction

Lipid molecules dissolved in water spontaneously form bilayer membranes, with properties very similar to those of biological membranes and vesicles [1]. The knowledge of the mechanics of vesicles started more than thirty years ago when both experimental and theoretical studies of amphiphilic bilayers engaged the attention of physicists and the interest of mathematicians [2]. In a viscous fluid, vesicles are drops a few tens of micrometers wide, bounded by impermeable lipid membranes a few nanometers thick. The membranes are homogeneous down to molecular dimensions; consequently, it is possible to represent the vesicle as a two-dimensional smooth surface in three-dimensional Euclidean space. Depending on the cases, the bilayers may be considered as liquid or solid.

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When liquid, the lipid molecules form a two-dimensional lattice and the membranes are described with an effective energy that does not penalize tangential displacements. Their mechanical properties permit a continuous mechanical description; such a deformable object is characterized by a flexion-governed membrane rigidity resulting from the curvature energy. The general theory accounts for surface strain, director extension, and director tilt associated with the misalignment of the surface normal. Galilean invariance is tantamount to the invariance of the energy under arbitrary two-dimensional orthogonal transformations and regarded as a function of a symmetric two-dimensional tensor. In this respect, the *Helfrich Hamiltonian*, which is quadratic in the curvature eigenvalues, provides a good description of lipid membranes and associates bending with an energy penalty [3–5]. Equilibrium configurations of the membrane satisfy a single normal 'shape' equation corresponding to the extrema of the Hamiltonian.
Fournier used a variational method to study fluid membranes [6]. Contrary wise, in this note, we revisit the mechanical behaviour of vesicle membranes by using the principle of virtual work [7–9] together with lemmas from the intrinsic differential geometry of surfaces; consequently, we do not need to use coordinate lines and Christoffel symbols associated with the membrane metric are useless here. For the Helfrich model, we established the equilibrium equation and the boundary conditions - which even apply to compressible media and extensible membranes on cell surfaces - as well as the condition on a surface/vesicle contact line [10–14]. For example, in the case of bending energy, we obtain the equilibrium equation of the vesicle, the conditions on surfaces and line when the vesicle is in contact with a solid boundary; the condition on the vesicle membrane yields the 'shape' equation and a modified Young-Dupré equation on the line.

The note is organized as follows:
In Section 2, we recall the principle of virtual work. Section 3 introduces universal geometrical tools associated with the notion of virtual displacements introduced in Section 2.1 and the Stokes formula for volumes, surfaces and lines. The variations of tensorial quantities and differential forms on surfaces and lines are proposed in an intrinsic form, with no representation in coordinate lines. Section 4 describes the vesicles' main background and the consequence it has on the variation of the vesicle's energy. A conclusion focusing on the advantage of the intrinsic geometrical method ends the note.

2 The principle of virtual work applied to continuous media

In continuum mechanics, the equilibrium of a medium can be studied with either the Newton model of *forces* or the Lagrange model of *work of forces.* At equilibrium, a minimization of the energy associated with a one-parameter family corresponds with the zero value of a linear functional of virtual displacements. The linear functional expressing the forces' work is related to the theory of distributions; a decomposition, associated with displacements considered as test functions whose supports are compact manifolds, uniquely determines a separated form respecting both the test functions and their transverse derivatives [15]. Then, the equilibrium equation and the boundary conditions are straightforwardly deduced from the principle of virtual work.

2.1 *The notion of virtual displacement*

The position of a continuous medium is classically represented by a transformation $\boldsymbol{\varphi}$ of a three-dimensional reference domain D_0 into the physical set D. In order to describe $\boldsymbol{\varphi}$ analytically, the variables $\boldsymbol{X} = (X^1, X^2, X^3)$ which single out individual particles in D_0 correspond to Lagrange's variables; the variables $\boldsymbol{x} = (x^1, x^2, x^3)$ in D correspond to Euler's variables. Transformation $\boldsymbol{\varphi}$ thus represents the position of a continuous medium,

$$\boldsymbol{x} = \boldsymbol{\varphi}\,(\boldsymbol{X}) \qquad \text{or} \qquad x^i = \varphi^i(X^1, X^2, X^3)\,,\ i \in \{1, 2, 3\}\,,$$

and possesses inverse and continuous derivatives up to the second order except on singular surfaces, curves or points. To formulate the principle of virtual work in continuum mechanics, we recall the notion of virtual displacements [16]: A one-parameter family of varied positions possessing continuous partial derivatives up to the second order and analytically expressed by the transformation

$$\boldsymbol{x} = \boldsymbol{\Phi}\,(\boldsymbol{X}, \eta)$$

with $\eta \in O$, where O is an open real set containing 0, and is such that $\boldsymbol{\Phi}\,(\boldsymbol{X},0) = \boldsymbol{\varphi}\,(\boldsymbol{X})$. The derivative, with respect to η at $\eta = 0$, is noted δ and is named *variation* [16] . In the physical space, the virtual displacement $\boldsymbol{\zeta}$ of a particle at $\boldsymbol{x}$ is such that $\boldsymbol{\zeta} = \delta\boldsymbol{x}$ when we assume $\delta\boldsymbol{X} = 0$ and $\delta\eta = 1$ at $\eta = 0$; the virtual displacement $\boldsymbol{\zeta}$ belongs to $T_{\boldsymbol{x}}(D)$, a tangent vector bundle to D at $\boldsymbol{x}$,

$$\boldsymbol{x} \in D \ \longrightarrow \boldsymbol{\zeta} = \boldsymbol{\psi}(\boldsymbol{x}) \equiv \frac{\partial \boldsymbol{\Phi}}{\partial \eta}\,|_{\eta=0} \in T_{\boldsymbol{x}}(D).$$

2.2 *The background underlying the principle of virtual work*

The virtual work of forces $\delta\tau$ is a linear functional value of the virtual displacement $\delta\boldsymbol{\varphi}$ determined by the variation of each particle and defined by

$$\delta\tau = < \Im, \delta\boldsymbol{\varphi} > \tag{1}$$

where $<\,,\,>$ denotes an inner product. In Relation (1), $\delta\boldsymbol{\varphi}$ is submitted to covector $\Im$ denoting all forces and stresses. Let us simply note that in case of motion, we must add the inertial forces, corresponding to the accelerations of masses, to the volume forces, and eventually add the viscous stresses to the conservative stress tensor. The virtual displacements are naturally submitted to the constraints resulting from constitutive equations such as mass

conservation for compressible media. In this case, the constraints are not necessarily expressed by Lagrange multipliers but are directly taken into account by virtual displacements submitted to the variations of the constitutive equations. Conversely, when geometrical assumptions are assumed, the Lagrange multipliers associated with geometrical conditions constrain the virtual displacements, which in all cases are named virtual displacements compatible with the constraints.
The principle of virtual work is expressed in the form : *For all virtual displacements compatible with the constraints, the virtual work of forces is null.*
If the distribution (1) is in a separated form [15], the principle of virtual work yields the equilibrium (or motion) equation and the boundary conditions [9].

3 Intrinsic geometrical tools for the energy of surfaces and lines

We assume that D has a differential boundary S, except on its edge C. We respectively note S_0 and C_0 the images of S and C in D_0; D and D_0 are Euclidian sets. The unit vector $\boldsymbol{n}$ and its image $\boldsymbol{n}_0$ are the oriented normal vectors to S and S_0; $c_m \equiv (R_m)^{-1}$ is the mean curvature of S; the vector $\boldsymbol{t}$ is the oriented unit vector to C and $\boldsymbol{n'} = \boldsymbol{t} \times \boldsymbol{n}$ is the unit binormal vector [17,18]. The tensor $\boldsymbol{F} \equiv \partial \boldsymbol{x}/\partial \boldsymbol{X}$ denotes the Jacobian transformation of $\boldsymbol{\varphi}$; symbols div, rot, tr and superscript ^{T} refer to the divergence, rotational, trace operators and the transposition, respectively; $\mathbf{1}$ denotes the identity tensor.

Lemma 1 *: we have the following relations*

$$\delta \det \boldsymbol{F} = \det \boldsymbol{F} \operatorname{div} \boldsymbol{\zeta}\,, \tag{2}$$

$$\delta\left(\boldsymbol{F}^{-1}\boldsymbol{n}\right) = -\boldsymbol{F}^{-1}\,\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{x}}\,\boldsymbol{n} + \boldsymbol{F}^{-1}\delta \boldsymbol{n}. \tag{3}$$

Proof of Rel. (2):

The Jacobi identity written in the form $\delta(\det \boldsymbol{F}) = \det \boldsymbol{F}\, \mathtt{tr}\left(\boldsymbol{F}^{-1}\delta \boldsymbol{F}\right)$ and

$$\delta \boldsymbol{F} = \delta\left(\frac{\partial \boldsymbol{x}}{\partial \boldsymbol{X}}\right) = \frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{X}},$$

imply,

$$\mathtt{tr}\left(\boldsymbol{F}^{-1}\delta \boldsymbol{F}\right) = \mathtt{tr}\left(\frac{\partial \boldsymbol{X}}{\partial \boldsymbol{x}}\,\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{X}}\right) = \mathtt{tr}\left(\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{X}}\,\frac{\partial \boldsymbol{X}}{\partial \boldsymbol{x}}\right) = \mathtt{tr}\left(\frac{\partial \boldsymbol{\zeta}}{\partial \boldsymbol{x}}\right) = \operatorname{div} \boldsymbol{\zeta}.$$

For an incompressible medium, $\det \boldsymbol{F} = 1$ and $\boldsymbol{\zeta}$ verifies

$$\operatorname{div} \boldsymbol{\zeta} = 0. \tag{4}$$

Proof of Rel. (3):

$$\delta\left(\boldsymbol{F}^{-1}\boldsymbol{n}\right) = \delta\left(\boldsymbol{F}^{-1}\right)\boldsymbol{n} + \boldsymbol{F}^{-1}\delta \boldsymbol{n}$$

and

$$\boldsymbol{F}^{-1}\,\boldsymbol{F} = \mathbf{1} \implies \delta\left(\boldsymbol{F}^{-1}\right)\boldsymbol{F} + \boldsymbol{F}^{-1}\,\delta\boldsymbol{F} = 0,$$

imply

$$\delta\left(\boldsymbol{F}^{-1}\right) = -\boldsymbol{F}^{-1}\,\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{X}}\boldsymbol{F}^{-1} = -\boldsymbol{F}^{-1}\,\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\ . \tag{5}$$

Lemma 2 *: The variation of $E = \iint_S \sigma\, ds$ is given by the relation*

$$\delta E = \iint_S \left[\delta\sigma - \left(\frac{2\sigma}{R_m}\,\boldsymbol{n}^T + \mathrm{grad}^{\mathrm{T}}\sigma\left(\mathbf{1} - \boldsymbol{n}\boldsymbol{n}^{\mathrm{T}}\right)\right)\boldsymbol{\zeta}\right] ds + \int_C \sigma\,\boldsymbol{n'}^T\boldsymbol{\zeta}\ dl. \tag{6}$$

where σ is a scalar field defined on S and ds, dl are the surface and the line measures.

Proof of Rel. (6):

The normal vector field is locally extended in the vicinity of S by the relation $\boldsymbol{n(x)} = \mathrm{grad}\ d(\boldsymbol{x})$, where d is the distance of point $\boldsymbol{x}$ to S; for any vector field $\boldsymbol{w}$,

$$\mathrm{rot}(\boldsymbol{n}\times\boldsymbol{w}) = \boldsymbol{n}\,\mathrm{div}\,\boldsymbol{w} - \boldsymbol{w}\,\mathrm{div}\,\boldsymbol{n} + \frac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}}\,\boldsymbol{w} - \frac{\partial\boldsymbol{w}}{\partial\boldsymbol{x}}\,\boldsymbol{n}.$$

From $\boldsymbol{n}^T\dfrac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}} = 0$ and $\mathrm{div}\,\boldsymbol{n} = -\dfrac{2}{R_m}$, we deduce on S,

$$\boldsymbol{n}^T\mathrm{rot}(\boldsymbol{n}\times\boldsymbol{w}) = \mathrm{div}\,\boldsymbol{w} + \frac{2}{R_m}\ \boldsymbol{n}^T\boldsymbol{w} - \boldsymbol{n}^T\frac{\partial\boldsymbol{w}}{\partial\boldsymbol{x}}\,\boldsymbol{n}. \tag{7}$$

Due to $E = \displaystyle\iint_S \sigma\ \det\left(\boldsymbol{n}, d_1\boldsymbol{x}, d_2\boldsymbol{x}\right)$ where $d_1\boldsymbol{x}$ and $d_2\boldsymbol{x}$ are two coordinate lines of S, we get,

$$E = \iint_{S_0} \sigma\ \det\boldsymbol{F}\ \det(\boldsymbol{F}^{-1}\boldsymbol{n}, d_1\boldsymbol{X}, d_2\boldsymbol{X}),$$

with $d_1\boldsymbol{x} = \boldsymbol{F}\,d_1\boldsymbol{X}$, $d_2\boldsymbol{x} = \boldsymbol{F}\,d_2\boldsymbol{X}$. Then,

$$\begin{aligned}\delta E = &\iint_{S_0} \delta\sigma\ \ \det\boldsymbol{F}\ \det\left(\boldsymbol{F}^{-1}\boldsymbol{n}, d_1\boldsymbol{X}, d_2\boldsymbol{X}\right)\\ &+ \iint_{S_0} \sigma\,\delta\big(\det\boldsymbol{F}\ \det\left(\boldsymbol{F}^{-1}\boldsymbol{n}, d_1\boldsymbol{X}, d_2\boldsymbol{X}\right)\big).\end{aligned}$$

Due to Lemma 1, $\boldsymbol{n}^T\dfrac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}} = 0$ and to $\boldsymbol{n}^T\delta\boldsymbol{n} = 0$,

$$\begin{aligned}&\iint_{S_0} \sigma\,\delta\big(\det\boldsymbol{F}\ \det\left(\boldsymbol{F}^{-1}\boldsymbol{n}, d_1\boldsymbol{X}, d_2\boldsymbol{X}\right)\big) =\\ &\iint_S \Big[\sigma\ \mathrm{div}\,\boldsymbol{\zeta}\ \ \det(\boldsymbol{n}, d_1\boldsymbol{x}, d_2\boldsymbol{x}) + \sigma\ \det\left(\delta\boldsymbol{n}, d_1\boldsymbol{x}, d_2\boldsymbol{x}\right)\\ &\qquad - \sigma\det\left(\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\,\boldsymbol{n}, d_1\boldsymbol{x}, d_2\boldsymbol{x}\right)\Big]\,ds =\\ &\iint_S \left(\mathrm{div}(\sigma\,\boldsymbol{\zeta}) - (\mathrm{grad}^T\sigma)\,\boldsymbol{\zeta} - \sigma\boldsymbol{n}^T\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\,\boldsymbol{n}\right) ds.\end{aligned}$$

Relation (7) yields

$$\operatorname{div}(\sigma\,\boldsymbol{\zeta})+\frac{2\sigma}{R_m}\,\boldsymbol{n}^T\boldsymbol{\zeta}-\boldsymbol{n}^T\frac{\partial(\sigma\,\boldsymbol{\zeta})}{\partial\boldsymbol{x}}\,\boldsymbol{n}=\boldsymbol{n}^T\operatorname{rot}(\sigma\,\boldsymbol{n}\times\boldsymbol{\zeta}).\qquad\text{Then,}$$

$$\iint_{S_0}\sigma\,\delta\big(\det\boldsymbol{F}\det(\boldsymbol{F}^{-1}\boldsymbol{n},d_1\boldsymbol{X},d_2\boldsymbol{X})\big)=$$
$$\iint_S\left(-\frac{2\sigma}{R_m}\,\boldsymbol{n}^T+\operatorname{grad}^T\sigma\,(\boldsymbol{n}\boldsymbol{n}^T-\mathbf{1})\right)\boldsymbol{\zeta}\,ds+\iint_S\boldsymbol{n}^T\ \operatorname{rot}(\sigma\,\boldsymbol{n}\times\boldsymbol{\zeta})\,ds,$$

where $\operatorname{grad}^T\sigma\,(\mathbf{1}-\boldsymbol{n}\boldsymbol{n}^T)\equiv\operatorname{grad}_{tg}^T\sigma$ belongs to the cotangent plane to S and

$$\iint_S\boldsymbol{n}^T\ \operatorname{rot}(\sigma\,\boldsymbol{n}\times\boldsymbol{\zeta})\,ds=\int_C(\boldsymbol{t},\sigma\,\boldsymbol{n},\boldsymbol{\zeta})\,dl=\int_C\sigma\,\boldsymbol{n'}^T\boldsymbol{\zeta}\ dl.$$

Then, we obtain relation (6).

Lemma 3 *: The variation of the internal energy is*

$$\delta\iiint_D\rho\ \alpha\,dv=\iiint_D(\operatorname{grad}p)^T\,\boldsymbol{\zeta}\,dv-\iint_S p\,\boldsymbol{n}^T\boldsymbol{\zeta}\,ds.\tag{8}$$

where ρ is the mass density, $\alpha(\rho)$ is the fluid specific energy, $p=\rho^2\dfrac{\partial\alpha}{\partial\rho}$ is the thermodynamical pressure [19] and dv is the measure of volume.

Proof of Rel. (8):

$\delta\iiint_D\rho\ \alpha\,dv=\iiint_D\rho\ \delta\alpha\,dv$ where $\delta\alpha=(\partial\alpha/\partial\rho)\ \delta\rho$. Due to mass conservation,

$$\rho\ \det\boldsymbol{F}=\rho_0(\boldsymbol{X}),\tag{9}$$

where ρ_0 is defined on D_0. The differentiation of Eq. (9) yields

$$\delta\rho\det\boldsymbol{F}+\rho\,\delta(\det\boldsymbol{F})=0,\ \text{and from Lemma 1, we get}$$

$$\delta\,\rho=-\rho\operatorname{div}\boldsymbol{\zeta}.$$

Consequently, $\operatorname{div}(p\ \boldsymbol{\zeta})=p\ \operatorname{div}\boldsymbol{\zeta}+(\operatorname{grad}p)^T\,\boldsymbol{\zeta}$ and we deduce relation (8).

In the same way,

Lemma 4 *: For any scalar field p defined on D,*

$$\delta\iiint_D p\ \operatorname{div}\boldsymbol{\zeta}\,dv=-\iiint_D(\operatorname{grad}p)^T\,\boldsymbol{\zeta}\,dv+\iint_S p\ \boldsymbol{n}^T\boldsymbol{\zeta}\,ds.\tag{10}$$

Lemma 5 *: The variation of the external unit vector normal to S is*

$$\delta\boldsymbol{n}=\left(\boldsymbol{n}\boldsymbol{n}^T-\mathit{1}\right)\left(\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\right)^T\boldsymbol{n}.\tag{11}$$

Proof of Rel. (11):

The property $\left\{\boldsymbol{n}^T d\boldsymbol{x} = 0 \Longrightarrow \boldsymbol{n}^T \boldsymbol{F}\, d\boldsymbol{X} = 0\right\}$ implies that vector $\boldsymbol{F}^T\boldsymbol{n}$ is normal to S_0 and consequently, $\boldsymbol{n}_0^T\,\boldsymbol{n}_0 = 1$ yields

$$\boldsymbol{n}_0 = \frac{\boldsymbol{F}^T\boldsymbol{n}}{\sqrt{(\boldsymbol{n}^T\boldsymbol{F}\boldsymbol{F}^T\boldsymbol{n})}}\,, \qquad \boldsymbol{n} = \frac{\boldsymbol{F}^{-1T}\boldsymbol{n}_0}{\sqrt{(\boldsymbol{n}_0^T\boldsymbol{F}^{-1}\boldsymbol{F}^{-1T}\boldsymbol{n}_0)}}\ .$$

Then, $\delta\boldsymbol{n}_0 = 0$ on the reference surface S_0 implies,

$$\delta\boldsymbol{n} = \frac{\delta\boldsymbol{F}^{-1T}\boldsymbol{n}_0}{\sqrt{\boldsymbol{n}_0^T\boldsymbol{F}^{-1}\boldsymbol{F}^{-1T}\boldsymbol{n}_0}} - \frac{1}{2}\,\boldsymbol{F}^{-1}\boldsymbol{n}_0\ \frac{\delta\left(\boldsymbol{n}_0^T\boldsymbol{F}^{-1}\boldsymbol{F}^{-1T}\boldsymbol{n}_0\right)}{\left(\boldsymbol{n}_0^T\boldsymbol{F}^{-1}\boldsymbol{F}^{-1T}\boldsymbol{n}_0\right)^{\frac{3}{2}}}\ .$$

From Eq. (5), $\delta\boldsymbol{F}^{-1T} = -\left(\dfrac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\right)^T\boldsymbol{F}^{-1T}$ and consequently,

$$\delta\boldsymbol{n} = -\left(\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\right)^T\boldsymbol{n} + \frac{1}{2}\,\boldsymbol{n}\left[\boldsymbol{n}^T\left(\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\right)\boldsymbol{n} + \boldsymbol{n}^T\left(\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\right)^T\boldsymbol{n}\right].$$

Then, $\boldsymbol{n}^T\left(\dfrac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\right)\boldsymbol{n} = \boldsymbol{n}^T\left(\dfrac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\right)^T\boldsymbol{n}$ implies relation (11).

Lemma 6 *: The variation of the mean curvature of S is*

$$\delta c_m = \frac{\partial c_m}{\partial\boldsymbol{x}}\,\boldsymbol{\zeta} + \frac{1}{2}\,\Delta_{tg}(\boldsymbol{n}^T\boldsymbol{\zeta}), \tag{12}$$

where Δ_{tg} is the tangential Beltrami-Laplace operator on surface S.

Proof of Rel. (12):

The variation of a derivative is given by

$$\delta\left(\frac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}}\right) = \frac{\partial\delta\boldsymbol{n}}{\partial\boldsymbol{x}} - \frac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}}\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}. \tag{13}$$

From $2\,c_m = -\operatorname{div}\boldsymbol{n} = -\operatorname{tr}\left(\dfrac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}}\right)$ and Eq. (13) we get,

$$2\,\delta c_m = -\operatorname{tr}\left(\frac{\partial\delta\boldsymbol{n}}{\partial\boldsymbol{x}}\right) + \operatorname{tr}\left(\frac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}}\frac{\partial\boldsymbol{\zeta}}{\partial\boldsymbol{x}}\right) = -\operatorname{div}\delta\boldsymbol{n} + \operatorname{div}\left(\frac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}}\,\boldsymbol{\zeta}\right) - 2\,\frac{\partial(\operatorname{div}\boldsymbol{n})}{\partial\boldsymbol{x}}\,\boldsymbol{\zeta}.$$

But, $\dfrac{\partial(\operatorname{div}\boldsymbol{n})}{\partial\boldsymbol{x}} = -2\dfrac{\partial c_m}{\partial\boldsymbol{x}}$ and by using Eq. (11) we get,

$$-\operatorname{div}\delta\boldsymbol{n} + \operatorname{div}\left(\frac{\partial\boldsymbol{n}}{\partial\boldsymbol{x}}\,\boldsymbol{\zeta}\right) = \operatorname{div}\left[\left(\boldsymbol{1} - \boldsymbol{n}\boldsymbol{n}^{\mathrm{T}}\right)\left(\frac{\partial\left(\boldsymbol{n}^{\mathrm{T}}\boldsymbol{\zeta}\right)}{\partial\boldsymbol{x}}\right)^{\mathrm{T}}\right] = \operatorname{div}\operatorname{grad}_{\mathrm{tg}}(\boldsymbol{n}^{\mathrm{T}}\boldsymbol{\zeta}),$$

and from $\operatorname{div}\operatorname{grad}_{\mathrm{tg}}(\boldsymbol{n}^T\boldsymbol{\zeta}) = \Delta_{tg}(\boldsymbol{n}^T\boldsymbol{\zeta})$ ([1]), we deduce relation (12).

[1] For all vector fields $\boldsymbol{x}\in D \to \boldsymbol{v}(\boldsymbol{x})$, $\operatorname{div}_{\mathrm{tg}}\boldsymbol{v} = \operatorname{div}\boldsymbol{v} - \boldsymbol{n}^{\mathrm{T}}(\partial\boldsymbol{v}/\partial\boldsymbol{x})\,\boldsymbol{n}$. Then, $\operatorname{div}_{\mathrm{tg}}\boldsymbol{v} = \operatorname{div}\boldsymbol{v} - \operatorname{tr}\left(\boldsymbol{n}\boldsymbol{n}^{\mathrm{T}}(\partial\boldsymbol{v}/\partial\boldsymbol{x})\right)$. But $\operatorname{div}\left(\boldsymbol{n}\boldsymbol{n}^{\mathrm{T}}\boldsymbol{v}\right) = \operatorname{div}\left(\boldsymbol{n}\boldsymbol{n}^{\mathrm{T}}\right)\boldsymbol{v} + \operatorname{tr}\left(\boldsymbol{n}\boldsymbol{n}^{\mathrm{T}}(\partial\boldsymbol{v}/\partial\boldsymbol{x})\right)$ and $\operatorname{div}\left(\boldsymbol{n}\boldsymbol{n}^{\mathrm{T}}\right) =$

4 Description of a vesicle membrane in contact with a solid surface

4.1 *Membranes' bending energy*

Vesicles consist in a three-dimensional domain bounded by a liquid bilayer. Vesicle interfaces are represented by material surfaces endowed with a bending surface energy. In our representation, a vesicle fills set D and lies on the surface of a solid; the vesicle is also surrounded by a fluid (see Fig. 1). All the interfaces between vesicle, solid and liquid are assumed to be regular. We note

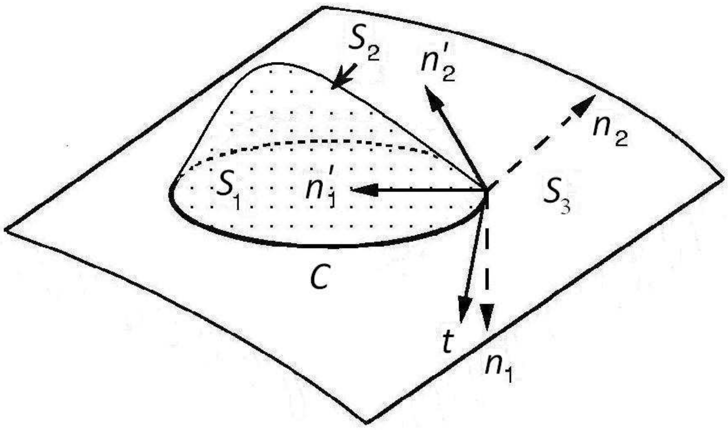

Fig. 1 A drop-shaped vesicle lies on a solid surface. The vesicle is bordered by a fluid (liquid) and a solid; S_1 is the boundary between liquid/solid; S_2 is the interface between vesicle/fluid (membrane of the vesicle); S_3 is the boundary between fluid/solid; $\boldsymbol{n}_1$ and $\boldsymbol{n}_2$ are the unit normal vectors to S_1 and S_2, external to the domain of the vesicle; contact line C is shared by S_1 and S_2 and $\boldsymbol{t}$ is the unit tangent vector to C relative to $\boldsymbol{n}_1$; $\boldsymbol{n'}_1 = \boldsymbol{n}_1 \times \boldsymbol{t}$ and $\boldsymbol{n'}_2 = \boldsymbol{t} \times \boldsymbol{n}_2$ are the binormals to C relative to S_1 and S_2, respectively.

σ_1, σ_2 and σ_3 the values of the surface energies of S_1, S_2 and S_3, respectively ([2]). The vesicle is submitted to a volume force $\rho\, \boldsymbol{f}$; $S = S_1 \cup S_2$ is the boundary of D; the external surface force on D is modelized with two vector fields $\boldsymbol{T}_1$ on the solid surface S_1 and $\boldsymbol{T}_2$ on the free vesicle surface S_2. In our calculus, the line tension on C is assumed to be null. Vector $\boldsymbol{n}$ stands for the normal to S external to D.

To obtain the equilibrium equation and the boundary conditions, it is neces-

div $(\boldsymbol{n})\, \boldsymbol{n}^{\mathrm{T}} + \boldsymbol{n}^{\mathrm{T}} \left(\partial \boldsymbol{n}/\partial \boldsymbol{x}\right)^{\mathrm{T}}$. From $(\partial \boldsymbol{n}/\partial \boldsymbol{x})\, \boldsymbol{n} = 0$ and $\mathrm{div}\boldsymbol{n} = -2/R_m$, we get $\mathrm{div}_{\mathrm{tg}}\boldsymbol{v} = \mathrm{div}\left((\mathbf{1} - \boldsymbol{n}\boldsymbol{n}^{\mathrm{T}})\, \boldsymbol{v}\right) - 2\, \boldsymbol{n}^{\mathrm{T}} \boldsymbol{v}/R_m$. From $\mathrm{div}_{\mathrm{tg}}\boldsymbol{v}_{\mathrm{tg}} = \mathrm{div}\boldsymbol{v}_{\mathrm{tg}}$ where $\boldsymbol{v}_{tg} = (\mathbf{1} - \boldsymbol{n}\boldsymbol{n}^T)\boldsymbol{v}$, we get $\mathrm{div}\, \mathrm{grad}_{\mathrm{tg}}(\boldsymbol{n}^{\mathrm{T}}\boldsymbol{\zeta}) = \mathrm{div}_{\mathrm{tg}}\, \mathrm{grad}_{\mathrm{tg}}\, (\boldsymbol{n}^{\mathrm{T}}\boldsymbol{\zeta}) = \Delta_{\mathrm{tg}}(\boldsymbol{n}^{\mathrm{T}}\boldsymbol{\zeta})$.

[2] Our aim is not to consider the thermodynamics of interfaces. Consequently σ_i, $i \in \{1, 2, 3\}$ are not taken into account as a function of variables like temperature or entropy.

sary to propose a constitutive behaviour for the membrane's energy density σ_2. As proved in the literature, the surface energy density on S_2 must be a function of the curvature tensor along the surface. To be intrinsic, σ_2 must be a function of the two curvature tensor invariants. If we note $c_1 = 1/R_1$ and $c_2 = 1/R_2$ the eigenvalues of the curvature tensor, the mean curvature and the Gauss curvature of S_2 are respectively noted,

$$H = \frac{c_1 + c_2}{2} = \frac{1}{R_m}, \qquad K = c_1\, c_2 = \frac{1}{R_1\, R_2}.$$

The external normal $\boldsymbol{n_2}$ to S_2 can be locally extended in the vicinity of S_2 by the relation $\boldsymbol{n_2}(\boldsymbol{x}) = \operatorname{grad} d_2(\boldsymbol{x})$, where d_2 is the distance of point $\boldsymbol{x}$ to S_2 (see Section 3, Lemma 2). Then,

$$2H = -\operatorname{div} \boldsymbol{n}_2 \equiv -\operatorname{tr}\left(\frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\right), \quad \frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}} = \left(\frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\right)^T, \quad \boldsymbol{n}_2{}^T \frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}} = 0, \quad (14)$$

$$2K = \left[\operatorname{tr}\left(\frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\right)\right]^2 - \operatorname{tr}\left(\frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\right)^2.$$

The surface's energy density σ_2 is assumed to be a regular function of H and K, but in the Helfrich model, the vesicle's surface energy is linear in K. The Gauss-Bonnet theorem ensures that the integration term corresponding to K is constant for closed surfaces, otherwise, the geodesic curvature of the boundary plays a role; this means, as established in [6], that the Gaussian curvature affects the boundary line actions. Nonetheless, experimental and theoretical studies have shown that the energy mainly stems from the bending [2]; consequently, in the Helfrich model, the surface energy density on S_2 is taken as a form without term in K:

$$\sigma_2 = \sigma_o + \frac{\kappa}{2}\left[2H - c_o\right]^2, \qquad (15)$$

where κ is the bending rigidity, c_o is the spontaneous curvature and σ_o is the superficial energy of capillarity. The main interest being the membrane's bending energy and its behaviour, we assume that the values of σ_o, σ_1 and σ_3 are constant. This special case can be easily extended, as done in [20] for an other problem of capillarity.

Lemma 7 *: The variation of the bending energy $E_2 = \iint_{S_2} \sigma_2\, ds$ of a membrane is* $\delta E_2 =$

$$\iint_{S_2}\left[\frac{d\sigma_2}{dn_2} - 2H\,\sigma_2 + \frac{1}{2}\,\Delta_{tg}\left(\frac{\partial \sigma_2}{\partial H}\right)\right]\boldsymbol{n}_2^T\boldsymbol{\zeta}\, ds + \int_C \boldsymbol{n}_2'^T\left(\sigma_2\,\boldsymbol{\zeta} + \boldsymbol{w}\right) dl, \quad (16)$$

where $\boldsymbol{w} = \dfrac{1}{2}\left[\dfrac{\partial \sigma_2}{\partial H}\ \operatorname{grad}_{\rm tg}(\boldsymbol{n}_2^T\boldsymbol{\zeta}) - \boldsymbol{n}_2^T\boldsymbol{\zeta}\ \operatorname{grad}_{\rm tg}\left(\dfrac{\partial \sigma_2}{\partial H}\right)\right]$ *and* $\dfrac{d}{dn_2} \equiv \left(\dfrac{\partial}{\partial \boldsymbol{x}}\right)\boldsymbol{n}_2$ *is the normal derivative in the direction $\boldsymbol{n}_2$.*

Proof of Rel. (16):

From Eq. (6), $\sigma_2 = \sigma_2(H)$ and Eq. (12), we obtain,

$$\delta E_2 = \iint_{S_2} \left[\frac{\partial \sigma_2}{\partial H} \frac{\partial H}{\partial \boldsymbol{x}} \boldsymbol{\zeta} + \frac{1}{2} \frac{\partial \sigma_2}{\partial H} \operatorname{div} \operatorname{grad}_{\mathrm{tg}}(\boldsymbol{n}_2^{\mathrm{T}} \boldsymbol{\zeta}) \right.$$
$$\left. - 2\, \sigma_2 H \boldsymbol{n}_2^{\mathrm{T}} \boldsymbol{\zeta} - \operatorname{grad} \sigma_2 \left(\mathbf{1} - \boldsymbol{n}_2 \boldsymbol{n}_2^{\mathrm{T}} \right) \boldsymbol{\zeta} \right] \mathrm{ds} + \int_{\mathrm{C}} \sigma_2\, \boldsymbol{n}_2'^{\mathrm{T}} \boldsymbol{\zeta}\, \mathrm{dl}$$

But, $\operatorname{grad} \sigma_2 = \dfrac{\partial \sigma_2}{\partial H} \dfrac{\partial H}{\partial \boldsymbol{x}}$; then,

$$\delta E_2 = \iint_{S_2} \left[\frac{1}{2} \frac{\partial \sigma_2}{\partial H} \operatorname{div} \operatorname{grad}_{\mathrm{tg}}(\boldsymbol{n}_2^{\mathrm{T}} \boldsymbol{\zeta}) + \left(\frac{d\sigma_2}{dn_2} - 2\, H \sigma_2 \right) \boldsymbol{n}_2^{\mathrm{T}} \boldsymbol{\zeta} \right] ds + \int_C \sigma_2 \boldsymbol{n}_2'^{T} \boldsymbol{\zeta}\, dl,$$

and from

$$\frac{1}{2} \frac{\partial \sigma_2}{\partial H} \operatorname{div} \operatorname{grad}_{\mathrm{tg}}(\boldsymbol{n}_2^{T} \boldsymbol{\zeta}) = \frac{1}{2} \mathit{\Delta}_{tg} \left(\frac{\partial \sigma_2}{\partial H} \right) \boldsymbol{n}_2^{T} \boldsymbol{\zeta} + \operatorname{div} \boldsymbol{w},$$

we deduce relation (16).

4.2 *Expression of the virtual work of forces*

For the Helfrich model, the total energy of the vesicle writes

$$\mathit{\Xi} = \iiint_D \rho\, \alpha(\rho)\, dv + \iint_{S_1} \sigma_1\, ds + \iint_{S_2} \sigma_2\, ds.$$

The virtual work of volume force $\rho \boldsymbol{f}$ defined on D writes $\iiint_D \rho\, \boldsymbol{f}^T \boldsymbol{\zeta}\, dv$. The virtual work of surface force $\boldsymbol{T}$ exerted on S is $\iint_S \boldsymbol{T}^T \boldsymbol{\zeta}\, ds$. Due to Eq. (6), $-\int_C \sigma_3\, \boldsymbol{n'}_1^T \boldsymbol{\zeta}\, dl$ corresponds to the action of S_3 on edge C. Finally, the virtual work of forces writes

$$\delta\tau = -\delta \mathit{\Xi} + \iiint_D \rho\, \boldsymbol{f}^T \boldsymbol{\zeta}\, dv + \iint_S \boldsymbol{T}^T \boldsymbol{\zeta}\, ds - \int_C \sigma_3\, \boldsymbol{n'}_1^T \boldsymbol{\zeta}\, dl. \qquad (17)$$

From Eqs. (6), (8), (16) and (17), we obtain

$$\begin{aligned} \delta\tau = & \iiint_D \left(\rho\, \boldsymbol{f}^T - \operatorname{grad}^T p \right) \boldsymbol{\zeta}\, dv \\ & + \iint_{S_1} \left[\left(p + \frac{2\, \sigma_1}{R_{m_1}} \right) \boldsymbol{n}_1^T + \boldsymbol{T}_1^T \right] \boldsymbol{\zeta}\, \mathrm{ds} \\ & + \iint_{S_2} \left\{ \left[p - \frac{d\sigma_2}{dn_2} + 2H\, \sigma_2 - \frac{1}{2} \mathit{\Delta}_{tg} \left(\frac{\partial \sigma_2}{\partial H} \right) \right] \boldsymbol{n}_2^T + \boldsymbol{T}_2^T \right\} \boldsymbol{\zeta}\, ds \\ & + \int_C \left[\left((\sigma_1 - \sigma_3)\, \boldsymbol{n'}_1^T - \sigma_2\, \boldsymbol{n'}_2^T \right) \boldsymbol{\zeta} - \boldsymbol{n'}_2^T\, \boldsymbol{w} \right] dl, \end{aligned} \qquad (18)$$

where $2/R_{m_1}$ is the mean curvature of S_1, and $\boldsymbol{T}_1$ and $\boldsymbol{T}_2$ correspond to the surface forces exerted on S_1 and S_2, respectively.

5 Equations governing equilibrium and boundary conditions

The fundamental lemma of variational calculus applied to each integral of Eq. (18) yields the equilibrium equation associated with domain D, the conditions on surfaces S_1 and S_2 and the condition on contact line C.

Equilibrium equation in D

$$\operatorname{grad} p = \rho\, \boldsymbol{f}.$$

This is the classical condition for equilibrium.

Condition on surface S_1

$$\left(p + \frac{2\,\sigma_1}{R_{m_1}}\right)\boldsymbol{n}_1 + \boldsymbol{T}_1 = 0.$$

Then $T_1 = -p_1\,\boldsymbol{n}_1$ is a normal stress vector to surface S_1 and we obtain the classical Laplace condition,

$$p_1 - p = \frac{2\,\sigma_1}{R_{m_1}}.$$

Condition on membrane surface S_2

$$\left[p - \frac{d\sigma_2}{dn_2} + 2H\,\sigma_2 - \frac{1}{2}\,\Delta_{tg}\left(\frac{\partial\sigma_2}{\partial H}\right)\right]\boldsymbol{n}_2 + \boldsymbol{T}_2 = 0. \tag{19}$$

Then, the stress vector must be normal to S_2. In fact $\boldsymbol{T}_2 = -p_2\,\boldsymbol{n}_2$ corresponds to the action of the external fluid on the membrane. From $\sigma_2 = \sigma_2(H)$, and taking Eq. (14) into account,

$$\frac{d\sigma_2}{dn_2} = \frac{\partial\sigma_2}{\partial H}\,\frac{dH}{dn_2} \quad \text{with} \quad 2\,\frac{\partial H}{\partial \boldsymbol{x}} = -\operatorname{div}\left(\frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\right)$$

and

$$2\,\frac{dH}{dn_2} \equiv 2\,\frac{\partial H}{\partial \boldsymbol{x}}\,\boldsymbol{n}_2 = -\operatorname{div}\left(\frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\right)\boldsymbol{n}_2 = -\operatorname{div}\left(\frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\,\boldsymbol{n}_2\right) + \operatorname{tr}\left(\frac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\right)^2.$$

Due to the fact that $\dfrac{\partial \boldsymbol{n}_2}{\partial \boldsymbol{x}}\,\boldsymbol{n}_2 = 0$, from Eq. (14) we get $\dfrac{dH}{dn_2} = 2\,H^2 - K$ and

$$\frac{d\sigma_2}{dn_2} = (2\,H^2 - K)\frac{\partial\sigma_2}{\partial H}.$$

Finally, Eq. (19) yields,

$$p - p_2 - (2\,H^2 - K)\frac{\partial\sigma_2}{\partial H} + 2H\,\sigma_2 - \frac{1}{2}\,\Delta_{tg}\left(\frac{\partial\sigma_2}{\partial H}\right) = 0. \tag{20}$$

In the case of the Helfrich model (15), we obtain from Eq. (20) the 'shape' equation ([3]):

$$p - p_2 + \kappa\,(2\,H - c_o)\left(2K - 2H^2 - c_o H\right) + 2\,H\,\sigma_o - 2\kappa\Delta_{tg}H = 0. \tag{21}$$

[3] Let us note that Helfrich *et al* [3–5] consider the vesicle as incompressible and the virtual displacement verifies $\operatorname{div}\boldsymbol{\zeta} = 0$ (see Eq. (4)). They assume that the lipid bilayer S has a

Condition on line C .

To get the line condition, we must consider a virtual displacement tangent to the fixed surface S_1 and consequently $\boldsymbol{\zeta} = \alpha\, \boldsymbol{t} + \beta\, \boldsymbol{t} \times \boldsymbol{n}_1$, where α and β are two scalar fields defined on C. From the last integral of Eq. (18), we get immediately: For any scalar field $\boldsymbol{x} \in C \longrightarrow \beta\,(\boldsymbol{x}) \in \Re$,

$$\int_C \left[\left(\,(\sigma_1 - \sigma_3)\, \boldsymbol{n'}^T_1 - \sigma_2 \boldsymbol{n'}^T_2\right)\boldsymbol{\zeta} - \boldsymbol{n'}^T_2 \boldsymbol{w}\right]\, dl = 0,$$

Due to the fact that $\boldsymbol{n}_2^T\, \boldsymbol{\zeta} = \beta\, \boldsymbol{n}_2^T\, (\boldsymbol{t} \times \boldsymbol{n}_1) = \beta\, \boldsymbol{t}^T\, (\boldsymbol{n}_1 \times \boldsymbol{n}_2) = \beta \sin\theta$, where $\theta = (\,\boldsymbol{n}_1, \boldsymbol{n}_2)$ is the Young angle, and the term $\beta \sin\theta$ is uniquely function of arc length l, we get $\boldsymbol{n'}^T_2 \operatorname{grad}_{\rm tg}(\beta\sin\theta) = 0$. Consequently, from Lemma 7,

$$\boldsymbol{n'}^T_2 \boldsymbol{w} = -\frac{1}{2}\left(\boldsymbol{n}_2^T\boldsymbol{\zeta}\right)\ \boldsymbol{n'}^T_2 \operatorname{grad}_{\rm tg}\left(\frac{\partial\sigma_2}{\partial H}\right) = -\frac{1}{2}\,\beta\sin\theta\,\sigma_2''(H)\,\frac{dH}{dn'_2},$$

where $\dfrac{dH}{dn'_2}$ is the value of the derivative of H along the line orthogonal to C on S_2. Consequently, $\forall\,\{l \longrightarrow \beta(l) \in \Re\}$,

$$\int_C \beta\left\{(\sigma_1 - \sigma_3)\,\boldsymbol{n'}^T_1(\boldsymbol{t}\times\boldsymbol{n}_1) - \sigma_2\boldsymbol{n'}^T_2(\boldsymbol{t}\times\boldsymbol{n}_1) + \frac{\sigma_2''(H)}{2}\,\frac{dH}{dn'_2}\sin\theta\right\}\ dl = 0.$$

Then,

$$\int_C -\beta\left\{(\sigma_1 - \sigma_3) + \sigma_2\boldsymbol{n}_2^T\boldsymbol{n}_1 - \frac{\sigma_2''(H)}{2}\,\frac{dH}{dn'_2}\sin\theta\right\}\ dl = 0,$$

and we obtain the line condition

$$(\sigma_1 - \sigma_3) + \sigma_2\cos\theta - \frac{\sigma_2''(H)}{2}\,\frac{dH}{dn'_2}\sin\theta = 0. \tag{22}$$

In the Helfrich model (15) the condition (22) yields

$$(\sigma_1 - \sigma_3) + \sigma_2\cos\theta - 2\,\kappa\,\frac{dH}{dn'_2}\sin\theta = 0. \tag{23}$$

Condition (23) replaces the classical Young-Dupré condition by taking additive term $-2\,\kappa\,\dfrac{dH}{dn'_2}\sin\theta$ into account.

total constant area S_0 and introduce the constraint $\iint_S ds = S_0$. Then, the virtual work is expressed as

$$\delta\tau = \iiint_D \rho\ \boldsymbol{f}^T\boldsymbol{\zeta}\ dv + \iint_S\ \boldsymbol{T}^T\boldsymbol{\zeta}\ ds - \delta\iint_S \sigma\ ds\ + \lambda_0\,\delta\iint_S ds + \delta\iiint_D p\ \operatorname{div}\,\boldsymbol{\zeta}\ \mathrm{dv},$$

where the scalar λ_0 is a constant Lagrange multiplier and p is a distributed Lagrange multiplier. Due to Eq. (10), the 'shape' equation that they deduced is identical to Eq. (21).

6 Conclusion and remarks

In this note, we propose simple systematic tools coming from surface geometry and from the principle of virtual work to obtain the boundary conditions on surfaces and lines for three-dimensional domains where the surfaces are endowed with surface energy densities. The tools are based on the Helfrich model with bending energy which is usually proposed to study the mechanics of biological membranes. The model does not take line energy into account, but the calculations will be similar to obtain the conditions at the boundaries of three-dimensional domains. Relation (6) is the key point of the model and highlights the extreme importance of knowing the variation of $\delta\sigma$ and consequently the behaviour of the surface energy σ. For example, in [20] we obtained a case where the capillary surface energy depended on the composition of the surface layer. The obtained results do not need to assume vesicle incompressibility and constant area of the membrane. We notice that the calculations proposed in the literature use the Christoffel symbols associated with coordinate curves on the surfaces, but the Christoffel symbols do not appear in the resulting expressions of the boundary conditions. This is an important reason for the straightforwardness of our method.

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